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On the Long-Range Exciton Transport in Molecular Systems: The Application to H-Aggregated Heterotriangulene Chains

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Abstract

© 2017 American Chemical Society. Self-assembled aggregates of pigment molecules are potential building blocks for excitonic circuits that find their application in energy conversion and optical signal processing. Recent experimental studies of one-dimensional heterotriangulene supramolecular aggregates suggested that singlet excitons in these structures can propagate on several micron distances. We explore this possibility theoretically by combining electronic structure calculations with microscopic models for exciton transport. A detailed characterization of the structural disorder and exciton decoherence is provided. We argue that advanced, well-established exciton transport models, used in our study, give about one order of magnitude shorter estimates for the exciton propagation length which suggest that there are other possible explanations of the experimental results.

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